

# Action principle for Numerical Relativity evolution systems

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A Lagrangian density is provided, that allows to recover the Z4 evolution system from an action principle. The resulting system is then strongly hyperbolic when supplemented by gauge conditions like '1+log' or 'freezing shift', suitable for numerical evolution. The physical constraint  $Z_\mu = 0$  can be imposed just on the initial data. The corresponding canonical equations are also provided. This opens the door to analogous results for other numerical-relativity formalisms, like BSSN, that can be derived from Z4 by a symmetry-breaking procedure. The harmonic formulation can be easily recovered by a slight modification of the procedure. This provides a mechanism for deriving both the field evolution equations and the gauge conditions from the action principle, with a view on using symplectic integrators for a constraint-preserving numerical evolution. The gauge sources corresponding to the 'puncture gauge' conditions are identified in this context.

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## I. INTRODUCTION

The role of action principles is so crucial in theoretical physics that its importance can not be overemphasized. In the case of the General Relativity, the standard action was proposed by Hilbert since the very beginning of the theory, although the Hamiltonian formulation had to wait for decades [1, 2]. The reason for this long delay is probably related to the complexity of the Cauchy problem for Einstein's equations, which becomes manifest in the 3+1 (space plus time) decomposition [2]. The coordinate gauge freedom produces a mismatch between the number of dynamical fields and that of true evolution equations: four of the field equations are indeed (energy-momentum) constraints. This rich structure opens the door to many different approaches.

On the other hand, by the end of the past century, some hyperbolic extensions of Einstein's equations were developed with a view on numerical relativity applications [3–6]. This emergent field is now more mature: there are two main formalisms currently used in numerical simulations. One is BSSN [7, 8], working at the 3+1 level, and the other is the class of generalized harmonic formalisms [9–11], working at the four-dimensional level. A unifying framework is provided by the Z4 formalism [12], which allows to recover the generalized harmonic one by relating the additional vector field  $Z_\mu$  with the harmonic 'gauge sources' [9]. On the other hand, it allows to recover (a specific version of) BSSN by a symmetry-breaking process in the transition from the four-dimensional to the three-dimensional formulations [13, 14].

There is a growing interest in incorporating the new hyperbolic formulations into the Lagrangian/Hamiltonian framework. An example is the usage of the 'densitized lapse' [3] as a canonical variable, leading to a modification in the standard form of the canonical evolution equations [15]. Reciprocally,

there are very recent attempts of modifying the ADM action in order to incorporate coordinate conditions of the type used in numerical relativity [16, 17], with a view on using symplectic integrators for the time evolution, which could ensure constraint preservation in numerical simulations [18]. On a different context, a well posed evolution formalism developed from a Lagrangian formulation could be a good starting point for Quantum Gravity applications.

In this paper we derive for the first time the Z4 formalism from an action principle by introducing a Lagrangian density which generalizes the Einstein-Hilbert one. We also provide the corresponding Hamiltonian, via the Legendre transformation. This is a crucial step towards the Hamiltonian formulation of other numerical-relativity formalisms, like BSSN. On the other hand, we recover the generalized harmonic formulations as usual, by relating the additional vector field  $Z_\mu$  with the harmonic 'gauge sources'. This mechanism is generalized, by identifying the gauge sources which correspond to the current numerical-relativity coordinate conditions, as we show explicitly for the 'puncture gauge': the combination of the '1+log' slicing and the gamma-driver conditions.

## II. THE ACTION PRINCIPLE

Let us consider the generic action

$$S = \int d^4x \mathcal{L} \quad (1)$$

with a Lagrangian density which generalizes the Einstein-Hilbert one by including an extra four-vector  $Z_\mu$ , namely

$$\mathcal{L} = \sqrt{g} g^{\mu\nu} [R_{\mu\nu} + 2 \nabla_\mu Z_\nu] \quad (2)$$

(we restrict ourselves to the vacuum case), with the Ricci tensor written in terms of the connection coefficients

$$R_{\mu\nu} = \partial_\rho \Gamma_{\mu\nu}^\rho - \partial_{(\mu} \Gamma_{\nu)\rho}^\rho + \Gamma_{\rho\sigma}^\rho \Gamma_{\mu\nu}^\sigma - \Gamma_{\sigma\mu}^\rho \Gamma_{\rho\nu}^\sigma, \quad (3)$$

(round brackets denote symmetrization).

Now let us follow the well-known Palatini approach, by considering independent variations of the metric density  $h^{\mu\nu} = \sqrt{g} g^{\mu\nu}$ , the connection coefficients  $\Gamma_{\mu\nu}^\rho$  and the vector  $Z_\mu$ . From the  $h^{\mu\nu}$  variations we get directly the Z4 field equations [12]

$$R_{\mu\nu} + \nabla_\mu Z_\nu + \nabla_\nu Z_\mu = 0, \quad (4)$$

which are currently used in many numerical-relativity developments [14].

From the  $\Gamma_{\mu\nu}^\rho$  and the  $Z_\mu$  variations we get a coupled set of equations which can be decomposed in a covariant way into the tensor equation

$$\nabla_\rho g^{\mu\nu} = 0, \quad (5)$$

which fixes the connection coefficients in terms of the metric, and the vector condition

$$Z_\mu = 0. \quad (6)$$

Let us note here the different role of the conditions (5) and (6). As there are much more independent connection coefficients than evolution equations in (4), we will consider condition (5) as a constraint enforcing the metric connection 'a posteriori', that is after the variation process. In this way, we will ensure that equations (4) are identical to the original Z4 equations, rather than some affine generalization. For this reason, we will assume a metric connection everywhere in what follows.

The case of condition (6) is different, as the Z4 equations (4) actually provide evolution equations for every component of  $Z_\mu$ . Then, (6) is a standard primary constraint and we have a choice among different strategies for dealing with it. If we enforce (6) into the Z4 field equations (4), we get nothing but Einstein's equations. This is not surprising because our Lagrangian obviously reduces to the Einstein-Hilbert one when  $Z_\mu$  vanishes. The problem is that the plain Einstein field equations do not lead directly to a well-posed initial data problem. This is why the original harmonic formulation [21–23] was used instead in the context of the Cauchy problem [24]. For the same reason, other formulations (BSSN [7, 8], generalized harmonic [9–11], Z4 [12, 13]) are currently considered in numerical relativity.

We can alternatively follow a different strategy. Instead of enforcing (6), we can deal with this condition as an algebraic restriction to be imposed just on the initial data, that is

$$Z_\mu|_{t=0} = 0 \quad (7)$$

In this way, we can keep the Z4 field equations which, when supplemented with suitable coordinate conditions, lead to a strongly hyperbolic evolution system [13, 14]. The consistency of this 'relaxed' approach requires that the constraint (6) should be actually preserved by the Z4 field equations (4). In this way, the solutions obtained

from initial data verifying (6) will actually minimize the proposed action (1).

Allowing for the conservation of the Einstein tensor, which is granted after the metric connection enforcement, we derive from (4) the second-order equation, linear-homogeneous in  $Z$

$$\nabla_\nu [\nabla^\mu Z^\nu + \nabla^\nu Z^\mu - (\nabla_\rho Z^\rho) g^{\mu\nu}] = 0. \quad (8)$$

It follows that the necessary and sufficient condition for the preservation of the constraint (6) is to impose also its first time-derivative conditions in the initial data, that is

$$(\partial_0 Z_\mu)|_{t=0} = 0. \quad (9)$$

Note that, allowing for (7) and the Z4 field equations, the secondary constraints (9) amount to the standard energy and momentum constraints, which are then to be imposed on the initial data in addition to (7).

This 'relaxed' treatment of the constraints (6) may look unnatural. But it is just the reflection of a common practice numerical relativity ('free evolution' approach), where four of the ten field equations (the energy-momentum constraints) are not enforced during the evolution, being imposed just in the initial data instead. The introduction of the extra four-vector in the Z4 formalism actually provides a simpler implementation of the same idea.

### III. HAMILTONIAN FORMALISM

A detailed look at the Lagrangian density (2) shows that the time derivatives of most of the variables are not present in  $\mathcal{L}$ . The only exceptions are the combinations

$$\Gamma_{\mu\nu}^0 - \delta_{(\mu}^0 \Gamma_{\nu)\rho}^\rho + 2\delta_{(\mu}^0 Z_{\nu)}. \quad (10)$$

This dynamical subset of variables can be decomposed into

$$\{ \Gamma_{ij}^0, Z_i - \frac{1}{2}(\Gamma_{ki}^k - \Gamma_{0i}^0), Z_0 - \frac{1}{2}\Gamma_{k0}^k \} \quad (i, j, k = 1, 2, 3), \quad (11)$$

The corresponding canonical momenta are given, respectively, by

$$\{ h^{ij}, 2h^{0i}, 2h^{00} \}. \quad (12)$$

The remaining quantities

$$\{ \Gamma_{\mu\nu}^k, \Gamma_{0\mu}^0 \} \quad (13)$$

can be considered as a sort of Lagrange multipliers, introducing constraints into the dynamical system, as their time derivatives do not enter the Lagrangian (see for instance ref. [19]).

Note that our Lagrangian (2) is linear in the time derivatives. This means that the relationship between field velocities and momenta can not be inverted. The

canonical momenta corresponding to (12, 13) vanish identically, and the ones corresponding to (11) coincide with the metric density components (12). This means that the Lagrangian (2) is a singular one: the corresponding (constrained) canonical formalism can be developed following the work of Dirac [20].

We will rather sketch here a simpler approach, by performing a limited Legendre transform, in the sense that it will only affect the dynamical subset (11), with canonical momenta (12). The remaining quantities will be considered as Lagrange multipliers, for which no Legendre transformation is required. We obtain in this way the Hamiltonian function

$$\mathcal{H} = -h^{\mu\nu} \{ \partial_k [ \Gamma_{\mu\nu}^k - \delta_\mu^k (\Gamma_{\rho\nu}^\rho - 2Z_\nu) ] + (\Gamma_{\rho\sigma}^\rho - 2Z_\sigma) \Gamma_{\mu\nu}^\sigma - \Gamma_{\sigma\mu}^\rho \Gamma_{\rho\nu}^\sigma \}, \quad (14)$$

where the metric densities are considered here as the canonical momenta associated to the dynamical fields (11).

The Hamilton equations for the fields (11) are precisely the Z4 equations (4). The Hamilton equations for their momenta (12) can be written as

$$\partial_\mu h^{\mu 0} = -h^{\mu\nu} \Gamma_{\mu\nu}^0 \quad (15)$$

$$\partial_\mu h^{\mu i} = -h^{\mu\nu} \Gamma_{\mu\nu}^i \quad (16)$$

$$\partial_0 h^{ij} = h^{ij} (\Gamma_{\rho 0}^\rho - 2Z_0) - 2 h^{\rho(i} \Gamma_{\rho 0}^{j)}, \quad (17)$$

which must be supplemented with the constraints derived from the Lagrange multipliers subset (13). A straightforward calculation shows that the full set of Hamilton equations is still equivalent to the Z4 equations (4), plus the metric connection requirement (5), plus the vanishing of  $Z_\mu$  (6). Indeed, allowing for (5, 6), the subsystem (15-17) is verified identically.

Note that in all our developments we have preserved general covariance. Our action integral (1) is a true scalar and, in spite of other alternatives, we have avoided the addition of total divergences which could have simplified our developments to some extent, at the price of adding boundary terms. This means that we keep at this point the full coordinate-gauge freedom.

This is reassuring from the theoretical point of view, but it can be a disadvantage if one is planning to use symplectic integrators for numerical evolution, as the required coordinate conditions must be supplied from the outside of the canonical formalism. This is why some recent works are trying to incorporate the coordinate conditions, via Lagrange multipliers, into the canonical framework [16, 17].

#### IV. GENERALIZED HARMONIC SYSTEMS

There is still another possibility, which allows a more direct specification of a coordinate gauge at the price of breaking the covariance of the evolution equations. which

are currently used in many numerical-relativity developments [14]. We can enforce in the Z4 equations (4) the following assignment for  $Z_\mu$

$$Z^\mu = -\frac{1}{2} \Gamma_{\rho\sigma}^\mu g^{\rho\sigma} \equiv -\frac{1}{2} \Gamma^\mu. \quad (18)$$

The vanishing of  $Z_\mu$  will amount in this way to the 'harmonic coordinates' condition, which can be considered then as a constraint to be imposed just in the initial data, that is

$$(\Gamma_{\rho\sigma}^\mu g^{\rho\sigma})|_{t=0} = 0 \quad (19)$$

(note that the extra field  $Z_\mu$  has disappeared in the process). The resulting field equations

$$R_{\mu\nu} - \partial_{(\mu} \Gamma_{\nu)} + \Gamma_{\mu\nu}^\rho \Gamma_\rho = 0 \quad (20)$$

lead, after imposing the metric connection condition (5), to the manifestly hyperbolic second-order system

$$g^{\rho\sigma} \partial_{\rho\sigma}^2 g_{\mu\nu} = 2 g^{\rho\sigma} g^{\alpha\beta} [\partial_\alpha g_{\rho\mu} \partial_\beta g_{\sigma\nu} - \Gamma_{\mu\rho\alpha} \Gamma_{\nu\sigma\beta}]. \quad (21)$$

This corresponds to the classical harmonic formulation of General Relativity [21–23], which is known to have a well-posed Cauchy problem [24].

We have derived in this way the harmonic formalism through the non-covariant prescription (18). The harmonic constraint (19) is automatically preserved by the resulting (harmonic) evolution system, provided that we also enforce the energy-momentum constraints on the initial data. This can be seen in a transparent way by replacing directly (18) into the covariant constraint-evolution equation (8) and then into the resulting conditions (9).

The prescription (18) can be generalized in order to enforce other coordinate gauges that are also currently used in numerical relativity. The simpler formulations [9, 11] correspond to the replacement

$$Z^\mu = -\frac{1}{2} (\Gamma^\mu + H^\mu), \quad (22)$$

where the 'gauge sources'  $H^\mu$  are explicit functions of the metric and/or the spacetime coordinates. More general choices of  $H^\mu$ , like that of ref. [25], would require a more elaborate treatment.

The same mechanism can be applied to coordinate conditions derived in the 3+1 framework, where the spacetime line element is decomposed as

$$ds^2 = -\alpha^2 dt^2 + \gamma_{ij} (dx^i + \beta^i dt) (dx^j + \beta^j dt). \quad (23)$$

The spacetime slicing is given by the choice of the time coordinate. In this context, the harmonic slicing condition can be generalized to [13]

$$(\partial_t - \beta^k \partial_k) \alpha = -f \alpha^2 \text{tr} K, \quad (24)$$

where  $K_{ij} = -\alpha \Gamma_{ij}^0$  stands for the extrinsic curvature of the time slices. The case  $f = 1$  corresponds to the

$\Gamma_{nnn} = 1/\alpha^2 (\partial_t - \beta^r \partial_r) \alpha$	$\Gamma_{nnk} = -\partial_k \ln \alpha$
$\Gamma_{knn} = 1/\alpha^2 \gamma_{kj} (\partial_t - \beta^r \partial_r) \beta^j + \partial_k \ln \alpha$	$\Gamma_{nij} = -K_{ij}$
$\Gamma_{ijn} = K_{ij} - 1/\alpha \gamma_{ik} \partial_j \beta^k$	$\Gamma_{kij} = {}^{(3)}\Gamma_{kij}$

TABLE I: The 3+1 decomposition of the four-dimensional connection coefficients. The index  $n$  is a shorthand for the contraction with the unit normal  $n_\mu$ .

harmonic time-coordinate choice, whereas the choice  $f = 2/\alpha$  corresponds to the popular '1+log' time slicing.

In order to get the replacement, of the form (22), which connects this condition with our formulation, we must rewrite (24) in a four-dimensional form with the help of the unit normal  $n_\mu$  to the constant time hypersurfaces, that is

$$n_\mu = \alpha \delta_\mu^0 \quad n^\mu = (-\delta_0^\mu + \delta_i^\mu \beta^i)/\alpha. \quad (25)$$

We can now decompose the four-dimensional Christoffel symbols in terms of the standard 3+1 quantities (see Table I). This provides a convenient way of translating 3+1 conditions like (24) in terms of four-dimensional objects.

We can obtain in this way, after an straightforward calculation, the gauge sources corresponding to the class of slicing conditions (24), namely

$$H^0 = (1 - 1/f) \Gamma_{\rho\sigma}^0 n^\rho n^\sigma. \quad (26)$$

We will use now (22) for replacing the quantity  $Z^0$  in the Z4 equations. Its evolution equation gets transformed in this way into a second order evolution equation for the lapse function  $\alpha$ , which governs the spacetime slicing. As the first-order slicing condition (24) has been translated into a specification of  $Z^0$ , and allowing for (8), (24) will become a first integral of the second order evolution system: we can impose it just in the initial data together with the energy-momentum constraints. This approach is new in 3+1 formalisms, but a common practice in the harmonic-like ones.

The same technique can be used for 'gamma-driver' shift prescriptions. A first-order reduction of the original 'gamma-freezing' condition [26] is given by [27]

$$(\partial_t - \beta^k \partial_k) \beta^i = \mu \tilde{\Gamma}^i - \eta \beta^i, \quad (27)$$

where  $\tilde{\Gamma}^i$  stands here for the contraction of the three-dimensional conformal connection, that is

$$\tilde{\Gamma}^i \equiv \gamma^{ij} \gamma^{rs} (\Gamma_{jrs} + \frac{1}{3} \Gamma_{rsj}). \quad (28)$$

The corresponding 'gamma-driver' gauge sources are given by

$$H_i = (1 - \frac{\alpha^2}{\mu}) \Gamma_{i\rho\sigma} n^\rho n^\sigma + \frac{1}{3} \Gamma_{\rho\sigma i} g^{\rho\sigma} \\ + (\frac{1}{3} - \frac{\alpha^2}{\mu}) \Gamma_{\rho\sigma i} n^\rho n^\sigma - \eta/\mu g_{0i}. \quad (29)$$

We can use again (22), this time for replacing the space vector  $Z_i$  in the Z4 equations. Its evolution equation get transformed in this way into a second order evolution equation for the shift components  $\beta^i$ , which determine the time lines. Again, the first-order gamma-driver condition (27) becomes a first integral of the resulting (second order) shift evolution equation. At the same time, one gets rid of the additional variables  $Z_i$  (as we did for  $Z^0$  with the analogous replacement, leading to the lapse evolution equation).

## V. CONCLUSIONS AND OUTLOOK

In summary, we are proposing the action (1), which generalizes the Einstein-Hilbert one. Starting from this action one gets directly the Z4 field equations, plus the metric connection condition (which is to be enforced 'a posteriori' in our Palatini approach), plus the constraints (6) stating the vanishing of  $Z_\mu$ . We have shown how a suitable treatment of these constraints allows working with the Z4 covariant evolution in the way one usually does in numerical relativity. The price to pay for this general-covariant approach is that closing the evolution system requires a separate coordinate gauge specification. The challenge is then to incorporate the evolution equations for the gauge-related quantities (lapse and shift) into the canonical formalism, either via Lagrange multipliers [16, 17] or by any other means.

We have also presented an alternative strategy, based in the 'gauge sources' approach, which characterizes the generalized harmonic formalisms. This allows to dispose of the additional  $Z_\mu$  vector field by enforcing at the same time the required coordinate conditions by means of some generalized gauge sources. The advantage of this second approach, at the price of getting a non-covariant evolution system, is that it can allow a direct use of symplectic integrators, devised to ensure constraint preservation during numerical evolution (see for instance ref. [18]). We have actually identified the gauge sources corresponding to some standard 3+1 gauge conditions, like the 'puncture gauge' consisting of the '1+log' lapse plus the gamma-driver shift prescriptions. The fact that these popular gauge conditions can fit into a Lagrangian/Hamiltonian approach, in the way we have shown, opens the door to new numerical relativity developments.

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